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Title: w19_OMEC Scientific Highlight

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w19_OMEC Scientific Highlight

❑ Scientific Achievement

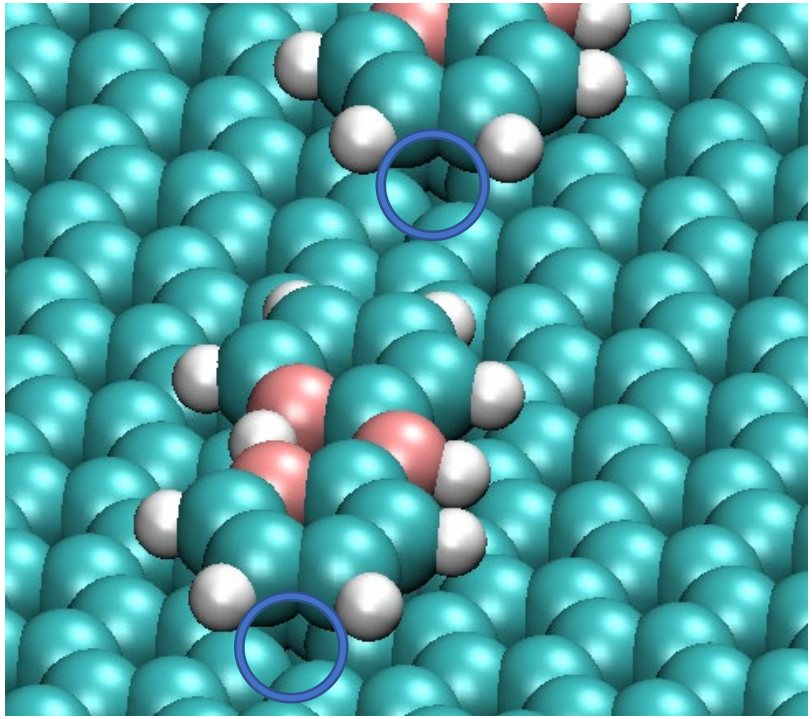
- Used DFT to identify likely experimental limitations for realizing high HER activity for DPA-based organic molecular electrocatalysts (OMEC) systems, directly guiding future experiments

❑ Significance and Impact

- OMECs promise low-cost, durable, systems for hydrogen production and energy applications
- Design of OMECs structures remain challenging due to lack of fundamental understanding
- Density functional theory (DFT) has been proposed to provide strong insights into HER activity
- DFT has identified non-graphitic/defected C as likely cause for low-activity found experimentally

❑ Research Details

- DFT calculations on the binding energy of HER intermediates for predicting reduction potentials and H adsorption energy as activity descriptors
- LANL Institutional Computing (HPC) Resources essential for successful execution of project for VASP and ADF calculations of HER descriptors



DPA+H on monovacancy (circles) containing graphene basal plane – this shifts H-binding energy descriptor from close to ideal to binding H ~1 eV too strongly.